

Angle-Resolved Photoemission Study of the Electronic Structures of AuAl_2 and PtGa_2

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INTRODUCTION

AuAl_2 and PtGa_2 are intermetallic compounds of both technological and scientific importance. The former has potential applications as a selective solar absorber [1], and the latter was proposed to be used as a thermodynamically stable conducting contact to GaAs [2]. They both crystallize in the fluorite structure, and superconduct at low temperatures [3]. They are also prototype materials for studying the Au and Pt 5d bands in intermetallic compounds, since group-III metals contribute only s-p states to the valence band (VB). The purple and gold colors of AuAl_2 and PtGa_2 , respectively, also strongly motivated researchers to study the electronic structures of these two compounds. Many electronic and physical properties of these two compounds have been measured, and a majority of these works was recently reviewed by Hsu [3]. However, no angle-resolved photoemission study of these two materials has been reported so far. This paper will focus on just such a study.

EXPERIMENTS

Procedures for preparation of the (100) and (111) faces of AuAl_2 and the (111) face of PtGa_2 were the same as those reported in a previous paper [4]. Experiments were carried out on beam line 7.0 at the Advanced Light Source. Photon energies in the range of 80 to 220 eV were selected with a low spherical grating monochromator, and a Perkin-Elmer 137-mm hemispherical analyzer was used in the fixed-analyzer-transmission mode to collect photoemission spectra. With 900 lines/mm for grating setting and 3 eV for analyzer pass-energy setting, the energy resolution of the photons plus the electrons was 0.15 eV as estimated from the sharpness of the Fermi edge of the VB photoemission spectra. The pressure during the measurement was 2×10^{-10} Torr. The vacuum chamber was also equipped with a double-anode (Al and Mg) x-ray source for x-ray photoemission spectroscopy (XPS) and x-ray photoelectron diffraction (XPD) measurements, and with a low-energy electron diffraction (LEED) system.

The samples were cleaned by repeated cycles of sputtering with Ar ions and annealing to 500°C until XPS spectra showed no traces of O or C contamination on the sample surfaces. The observed XPD and LEED patterns also confirmed the cleanliness and ordering of the respective surfaces.

RESULTS AND DISCUSSION

Figs. 1 and 2 show a set of VB photoemission spectra from the (100) and (111) faces, respectively, of AuAl_2 , and Fig. 3 shows that from the (111) face of PtGa_2 at normal emission. The photon energy ($h\nu$) was varied so as to probe the third to the fourth Brillouin zone (BZ) for the (100) face, and the fourth to the fifth BZ for the (111) face. The Fermi energy (E_F) was assigned at half height on the onset of a plateau, which is caused by photoemission from the Au or Pt s-p band. In general, the s-p bands disperse much more rapidly than the d bands, which accounts for the differing relative widths of the features seen in the photoemission spectra. For PtGa_2 , there is a three-peak structure at higher binding energy (E_B) with mainly Pt 5d character. The crystal-field and spin-orbit parameters of PtGa_2 were determined to be 0.90 and 0.56 eV, respectively, in the same manner as was done in Ref. [4]. We note that the E_B values at the three

Γ points (at approximately $h\nu=110$ or 220 eV) for PtGa_2 are 3.40, 4.35, and 5.45 eV, which are essentially the same as those obtained from the density-of-states (DOS) features in the angle-integrated photoemission spectra [4]. This means that the Pt 5d bands in PtGa_2 are well localized and do not disperse more than 0.3 eV. We should also point out that these E_b values are within 10% of the corresponding values for elemental Au [5], which explains why PtGa_2 is gold-colored.

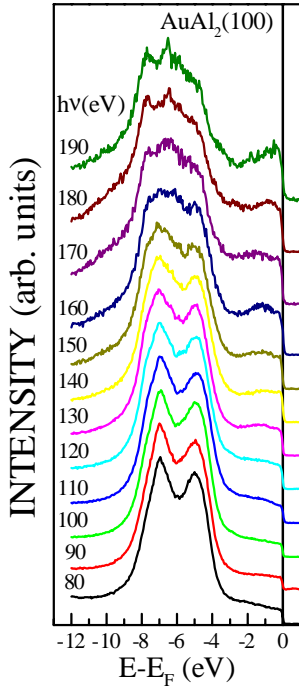


Figure 1. Angle-resolved photoemission spectra from the (100) face of AuAl_2 taken at normal emission.

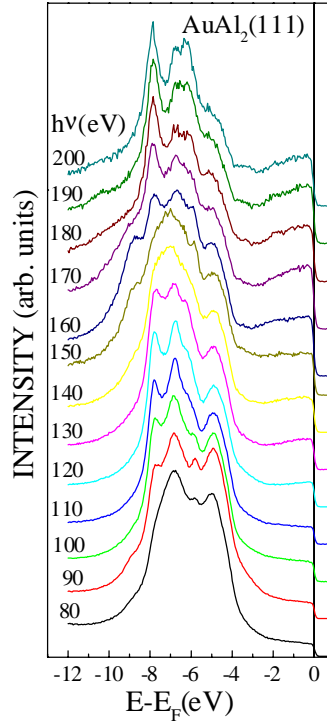


Figure 2. Angle-resolved photoemission spectra from the (111) face of AuAl_2 taken at normal emission.

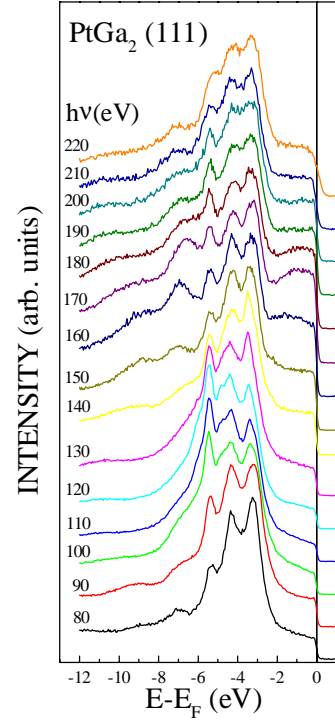


Figure 3. Angle-resolved photoemission spectra from the (111) face of PtGa_2 taken at normal emission.

By using a direct-transition model and assuming a free-electron conduction-band structure [6], the E vs. k curves can be plotted. The values of the inner potential used for AuAl_2 and PtGa_2 were estimated to be 12.1 and 10.8 eV, respectively. These values were taken to be the differences between the muffin-tin zeros of energy in the augmented-plane-wave calculations [7,8] and the vacuum level as determined from the work functions of the two compounds. In Fig. 4, the experimentally derived bands of AuAl_2 are compared with the bands obtained from a nonrelativistic band-structure calculation [7], while in Fig. 5, those of PtGa_2 are compared with the bands obtained from a semi-relativistic band-structure calculation [8]. The agreement between experiment and theory is very poor for AuAl_2 , but rather good for PtGa_2 , which indicates that the spin-orbit effect is important in calculating the band structures of these materials. The experimental band for PtGa_2 at roughly $E_b=7$ eV (indicated by diamonds in Fig. 5) probably involves the one-dimensional DOS effect [9], while that at roughly $E_b=4.7$ eV (indicated by squares in Fig. 5) probably involves a surface state.

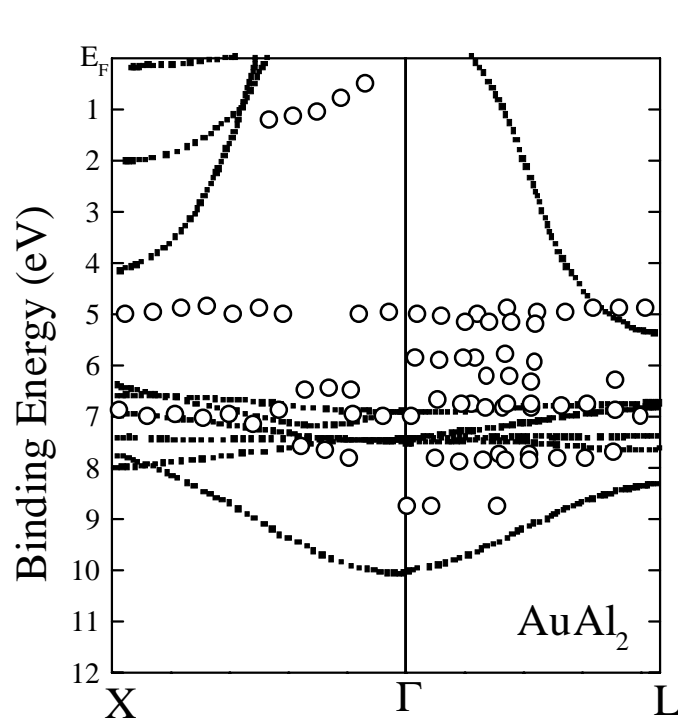


Figure 4. Band structure of AuAl_2 along X- Γ -L. Open circles are experimental dispersion curves.

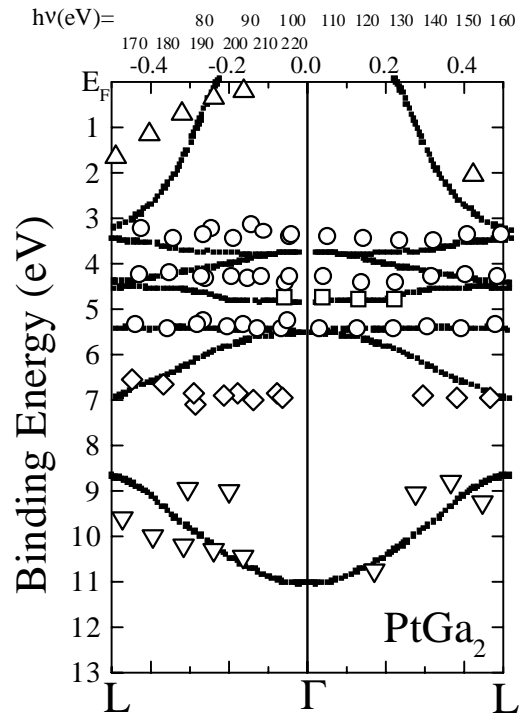


Figure 5. Band structure of PtGa_2 along Γ -L. Open circles, squares, diamonds, and triangles are experimental dispersion curves.

ACKNOWLEDGMENTS

We thank R.J. Baughman and R.S. Williams for supplying the samples.

REFERENCES

1. R.E. Hahn and B.O. Seraphin, Phys. Thin Films **10**, 1 (1978).
2. Y.K. Kim, D.A. Baugh, D.K. Shuh, R.S. Williams, L.P. Sadwick, and K.L. Wang, J. Mater. Res. **5**, 2139 (1990).
3. L.-S. Hsu, Mod. Phys. Lett. B **8**, 1297 (1994), and references therein.
4. L.-S. Hsu and K.-L. Tsang, Phys. Rev. B **56**, 6615 (1997).
5. K.A. Mills, R.F. Davis, S.D. Kevan, G. Thornton, and D.A. Shirley, Phys. Rev. B **22**, 581 (1980).
6. J.G. Nelson, W.J. Gignac, S. Kim, J.R. Lince, and R.S. Williams, Phys. Rev. B **31**, 3469 (1985).
7. A.C. Switendick and A. Narath, Phys. Rev. Lett. **22**, 1423 (1969).
8. K.J. Kim, B.N. Harmon, L.-Y. Chen, and D.W. Lynch, Phys. Rev. B **42**, 8813 (1990).
9. T. Grandke, L. Ley, and M. Cardona, Phys. Rev. B **18**, 3847 (1978).

This work was supported by the National Science Council, Taiwan, R.O.C., the U.S. Department of Energy under Contract No. DE-FG-02-90ER45416, and the U.S. National Science Foundation under Contract No. DMR-94-23741.

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